

1-Hexanol
111-27-3 | DTXSID8021931

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.24×10^{-11} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.76×10^{-1}

Confidence level: 9.82×10^{-1}

Nearest Neighbors from the Training Set

Image not found

1-Hexanol

Measured: 1.25×10^{-11}

Predicted: 1.24×10^{-11}

Image not found

Isopentyl alcohol

Measured: 1.31×10^{-11}

Predicted: 1.25×10^{-11}

Image not found

Pentan-2-ol

Measured: 1.18×10^{-11}

Predicted: 1.20×10^{-11}

Image not found

3-Pentanol

Measured: 1.22×10^{-11}

Predicted: 1.20×10^{-11}